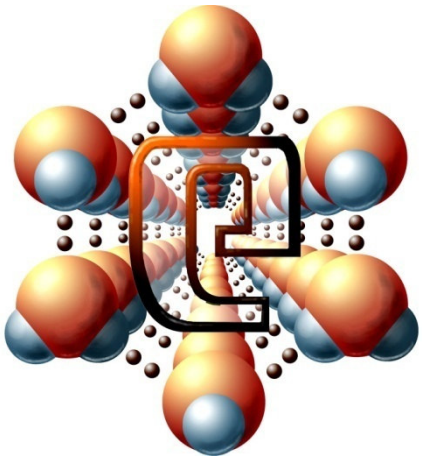


Bloch wave Simulator

User's Manual

v. 1.0

February 2009

Visit our web-page at: www.analitex.com

Table of Contents

1 Preface

This preface provides information about the *Bloch wave Simulator User's Manual* and links to AnaliteX technical support.

1.1 General introduction

Bloch Simulator is a program which allows you to calculate and visualize dynamical Convergent Beam Electron Diffraction (CBED) patterns by the Bloch wave method.

1.2 Support offerings

You can always contact AnaliteX at **support@analitex.com**to find out how the *Bloch wave Simulator* program can meet your needs and for technical support.

1.3 Reporting problems

If you can have problems while running *Bloch wave Simulator* or any of its components, please report them to the AnaliteX support team by email (**support@analitex.com**).

2 Installing *Bloch wave Simulator*

Bloch wave Simulator runs under Windows® 2000, XP or Vista, and is usually included as an optional component in the eMap software package.

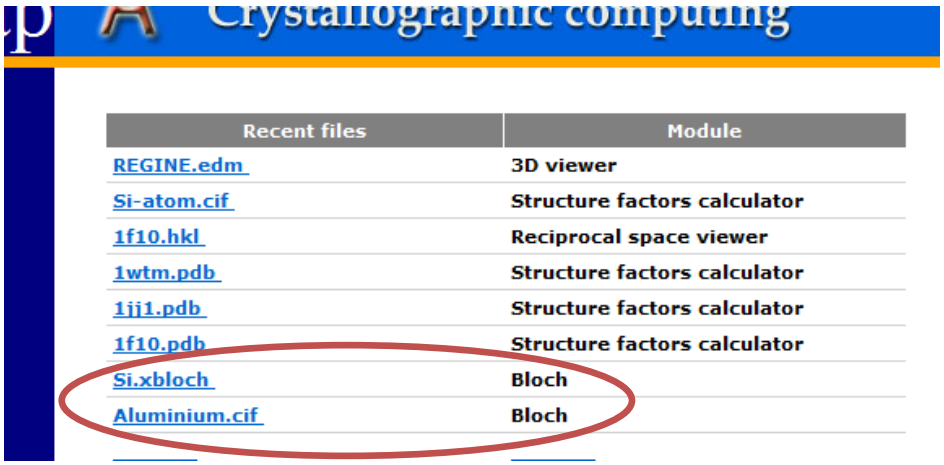
2.1 Installation

Install the program by clicking on **Setup.exe** located in the directory **eMap** on the CD. The program will ask you to choose destination location, the default is **C:\Program Files\AnaliteX\eMap**. Use **Browse** if you want to put the program in another directory, or on another drive. Click **Next** when the program folder and drive are as required. Then you will be asked to select program folders under which eMap is run from the Start menu. Select the program folder (default = **eMap**) and click on **Finish**.

2.2 User interface

The *Bloch wave Simulator* module can be initiated from the **Start page**. **NOTE**: This page will only appear if the ***MS Internet Explorer*** is installed. In the case when eMap fails to locate the

Internet Explorer, a simplified **Installed components** dialog will appear.



The modules browser is a page with image buttons representing each available module. A short description text is displayed on the right side when you select the button using a mouse. To launch a required component, click on the short description text on the right side of the corresponding image button.

The *Bloch wave Simulator* can be launched by pressing on the  button on the Start Page or choosing a link to a recently used file.

3 Bloch Wave Simulator

The *Bloch wave Simulator* module is designed for the calculation and visualization of Convergent Beam Electron Diffraction (CBED) dynamical electron diffraction patterns.

The Bloch wave method:

- conforms to calculations of diffraction patterns of structures with small unit cell parameters;
- is fast with high accuracy for a perfect crystal in a <*u*,*v*,*w*> direction with low symmetry i.e. small number of beams;
- calculates CBED patterns in any <*u*,*v*,*w*> direction.

3.1 Brief description of the Bloch wave theory

The time-independent wave equation (Helmholtz equation or elliptic partial differential equation) is:

where Ψ is the wave function, K_0 is the relativistic wave number in the form of 1/λ and

$$U(\boldsymbol{r}) = \frac{\sigma}{\pi\lambda} V(\boldsymbol{r})$$

with σ as the interaction constant and $V(\boldsymbol{r})$ as the electrostatic (lattice) potential.

The lattice potential can be expanded into a Fourier series and the electron wave inside the crystal for an arbitrary wave vector $\boldsymbol{k}$ can be written as a Bloch wave,

$$\Psi(\boldsymbol{r}) = \sum_g C_g e^{2\pi \mathrm{i}(\boldsymbol{g}+\boldsymbol{k})\boldsymbol{r}},$$

where C_g are called Bloch wave coefficients.

Substituting $\Psi(\boldsymbol{r})$ into the wave equation gives the following form,

$$\sum_g \left[\{k_0^2 - (\boldsymbol{k}+\boldsymbol{g})^2\}C_g + \sum_{h\neq g} U_{g-h}C_h\right] e^{2\pi i(\boldsymbol{g}+\boldsymbol{k})\boldsymbol{r}} = 0,$$

or

$$\{k_0^2 - (\boldsymbol{k}+\boldsymbol{g})^2\}C_g + \sum_{h\neq g} U_{g-h}C_h = 0.$$

This equation can be represented in a matrix form as followed,

$$\begin{bmatrix} k_0^2 - \boldsymbol{k}^2 & U_{0-g} & \cdots & U_{0-h} & \cdots & U_{0-m} \\ U_{g-0} & k_0^2 - (\boldsymbol{k}+\boldsymbol{g})^2 & \cdots & U_{g-h} & \cdots & U_{g-m} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ U_{h-0} & U_{h-g} & \cdots & k_0^2 - (\boldsymbol{k}+\boldsymbol{h})^2 & \cdots & U_{h-m} \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ U_{m-0} & U_{m-g} & \cdots & U_{m-h} & \cdots & k_0^2 - (\boldsymbol{k}+\boldsymbol{m})^2 \end{bmatrix} \begin{bmatrix} C_0 \\ C_g \\ \vdots \\ C_h \\ \vdots \\ C_m \end{bmatrix} = 0.$$

The final problem can be solved using matrix diagonalization to determine the wave vectors, $\boldsymbol{k}$, and all the Bloch coefficients, C_g.

The *Bloch wave Simulator* uses an optimized diagonalization functions from Intel® Math Kernel Library (Intel® MKL).

3.2 Speed of calculations

The calculation speed depends on several parameters which are described below.

Parameter	Description
g_{max}	Limits the total resolution of the simulated diffraction pattern. Reflections with $g_{hkl} > g_{max}$ will not be included in the calculations.
$S_{g,max}$	Maximum value for the excitation error, S_g. Limits the number of exact beams.
$S_{g,Bethe}$	Maximum value for the excitation error, S_g. Limits the number of Bethe beams.
HOLZ layers	Maximum number of HOLZ layers to include in the calculations.
Voltage	At low voltages more HOLZ reflections can fall within g_{max}.
Number of points	Every disk, line etc. will be digitized with resolution equal to the specified number of points. For example, in case of the CBED disk the number of points N_{points} corresponds to the

	CBED disk diameter. In this case the total number of points inside every CBED disk would be **round**($\pi \cdot N_{points}^2$).

NOTE: The total number of beams N produces a matrix of size N*N with complex numbers of double precision as matrix elements. With N=300, the memory requirements for the matrix storage will be ~1.4 Mb. The time needed to diagonalize a matrix with N=300 may vary depending on the processor's speed. For Intel® Core2 Quad this time is less than 1 second ***per diagonalization***. However, increasing the number of beams can significantly increase the calculation time. Note that in the case of a CBED disk the single matrix diagonalization time will be multiplied by the number of pixels inside the disk. For example a typical CBED pattern of a simple silicon crystal structure in the [111] zone axis orientation with a CBED disk size of 16 pixels would take about 20-30 sec to calculate on the Intel® Core2 Quad processor.

3.3 Limiting number of beams

There are several options which can speed up the calculations, especially in the case when the type of calculations is set to the CBED disk with a large number of points.

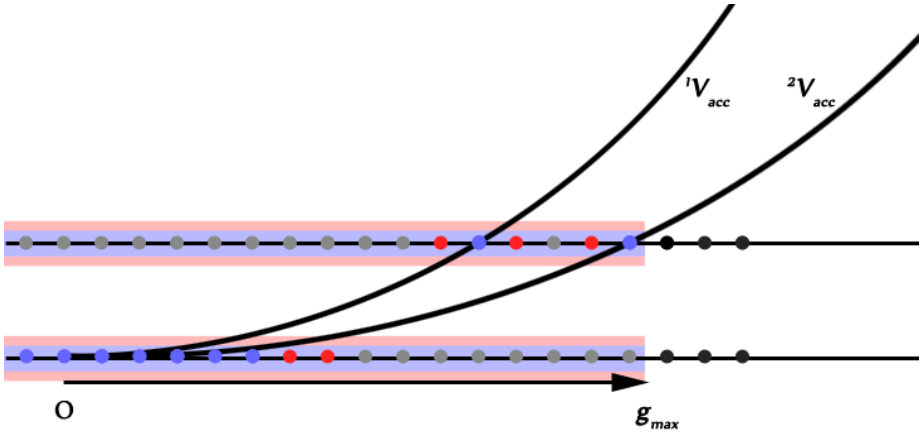


Figure. The geometry of the Bloch wave calculations

(see text for explanations).

Voltage. The curvature of the Ewald sphere increases with lower accelerating voltage values ($^1V_{acc} < {}^2V_{acc}$). Decreasing the voltage can increase the total number of reflections, provided that other parameters remain unchanged.

$S_{g,max}$*.** Increasing $S_{g,max}$ will increase the number of reflections, which will be counted as *exact* (blue area around the reciprocal layers on ***Figure) and will participate in the matrix diagonalization.

$S_{g,Bethe}$*.** Increasing $S_{g,Bethe}$ will increase the number of reflections, which will be counted as *Bethe* (red area around the reciprocal layers on ***Figure) and will participate only in *Generalized Bethe Approximation*.

Number of points. The total number of matrix diagonalizations in the case of CBED disk calculation mode can be approximately evaluated by the following equation:

$$N_{total} = round\left(\pi \cdot N_{points}^2\right) \cdot N_{beams}.$$

where N_{beams} is the total number of the exact beams in the diffraction pattern. In the case of other calculation types the N_{total} will vary.

HOLZ layers. Changing the number of HOLZ layers will increase the total number of reflections within the given $\boldsymbol{g_{max}}$ value.

3.4 Calculations type

There are several calculation types available in the *Bloch wave Simulator*:

1. **Point.** The dynamical diffraction pattern will be calculated as a point (spot or regular) diffraction pattern.
2. **CBED disk.** The dynamical diffraction pattern will be calculated as a disk diffraction pattern.
3. **Rectangle.** The dynamical diffraction pattern will be calculated as a diffraction pattern with rectangular reflections.
4. **Circle.** The dynamical diffraction intensities will be calculated only along every disk, forming circles with

empty centres similar to a TEM DIFF mode with the rocking beam on and ***without descan***. The width (pixels) of the circle stroke and circle radius (pixels) can be specified in the *Bloch Settings Panel*.

5. **Precession.** This calculation mode is similar to the **Circle** mode except that after the calculations the intensities will be averaged along the circle. The pattern will be displayed as a regular dynamical spot precession electron diffraction pattern similar to a TEM DIFF mode with rocking beam on and ***with descan***. The width (pixels) of the circle stroke and circle radius (pixels) can be specified in the *Bloch Settings Panel*

6. **LACBED.** This calculation mode is similar to **CBED** mode except only the *000* reflection will be shown.

7. **Line.** In this calculation mode a line segment of a CBED disk will be calculated. The line slope (degrees), length (pixels) and width (pixels) can be specified in the *Bloch Settings Panel*.

4 Supported file formats

Bloch wave Simulator supports several input data file types.

4.1 Native format XBLOCH

The native format of the *Bloch wave Simulator* is the XML file format with custom file extension *.*xbloch*. The *Bloch wave Simulator* will automatically generate files in this format and prompt for the user's permission to save before exit from the program.

The XBLOCH XML files contain the entire *Bloch wave Simulator* settings and Bloch wave calculated data, if any calculations were performed.

A XBLOCH file contains the complete crystallographic information about the loaded crystal needed for Bloch wave calculations. This crystallographic data includes:

- the symmetry (*space group* number and *extension*);
- the unit cell parameters;
- information about unique atoms (chemical element name, *xyz* fractional coordinates, occupancies and temperature factors).

4.2 Crystallographic file types

The *Bloch wave Simulator* can load files which contain crystallographic information such as symmetry, unit cell and atomic positions. The file types are SHELX *INS*, *CIF*, *XYZ*, *TXT* (see the ***eMap manual***), *AT* and *PDB*.

5 The user interface

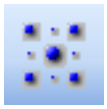
The *Bloch wave Simulator* has several ways for data handling and calculations. The following sections will describe the available commands in details.

5.1 The toolbar

There is one extra toolbar available in the *Bloch wave Simulator*:

Description	Toolbar button
Run. Starts the Bloch wave calculations. This button can be ***disabled*** when the *Bloch wave Simulator* finished the calculations or a file with Bloch calculations was loaded. In order to ***restart*** press the **Create new document** button ().	
Crystal structure view. Switches to the structure preview mode (in the current zone axis orientation).	

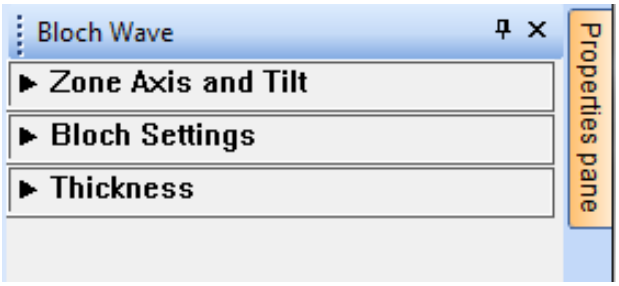
Diffraction pattern view. Switches to the simulated diffraction pattern preview mode.



Colour control. Shows the colour control dialog in order to change the values of gamma/contrast/brightness of the calculated electron diffraction pattern.

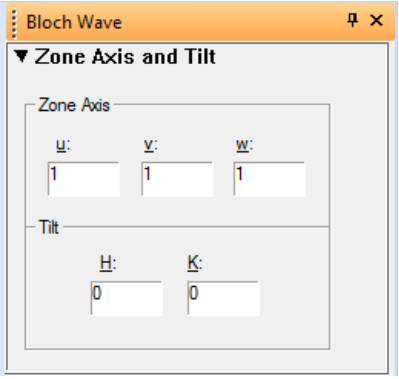
5.2 Side panel dialog bar.

Bloch Simulator offers a 3-panel dialog bar on the right side (default) of the main view. This bar can be relocated to any side of the current view or the main window (left or right sides are preferable due to the vertical nature of the dialog bar items placement). Any dialog panel can be hidden or closed any time by using the 2 respective buttons  in the top-right corner of the bar.



The side panel **Dialog** bar

5.2.1 The Zone Axis and Tilt dialog panel

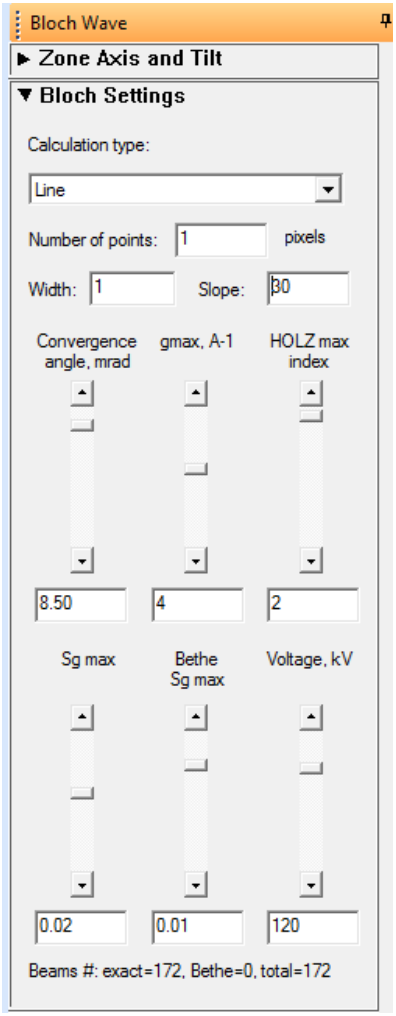


The **Zone Axis and Tilt** dialog panel.

The **Zone Axis and Tilt** dialog panel allows the user to control the current zone axis indices and the tilt away from the zone axis (within values of 2D plane *hk* indices).

These controls may be disabled if the Bloch data was calculated. In order to reset the data and be able to modify the zone axis and tilt press the **Create new document** button ().

5.2.2 The Bloch Settings dialog panel



The **Bloch Settings** dialog panel.

The **Bloch Settings** dialog panel allows the user to control the current settings for the Bloch wave calculations.

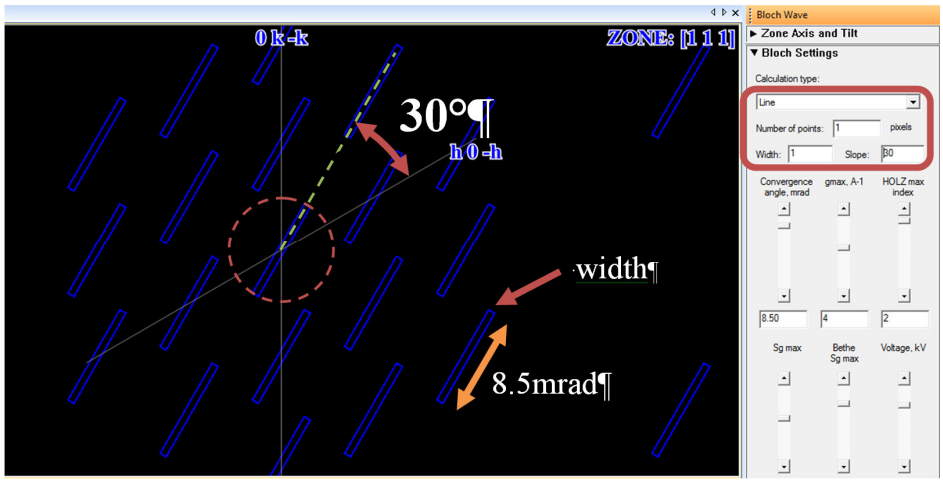
If the calculations type is ***Point*** then the ***Number of points*** edit box will be set to 1 and disabled automatically.

These controls may be disabled if the Bloch data was calculated. In order to reset the data and be able to modify controls press the **Create new document** button ().

For the ***Line*** calculation mode the line ***Width*** (in *mrad*) and the ***Slope*** (in degrees) to the a-axis of the diffraction pattern can be modified.

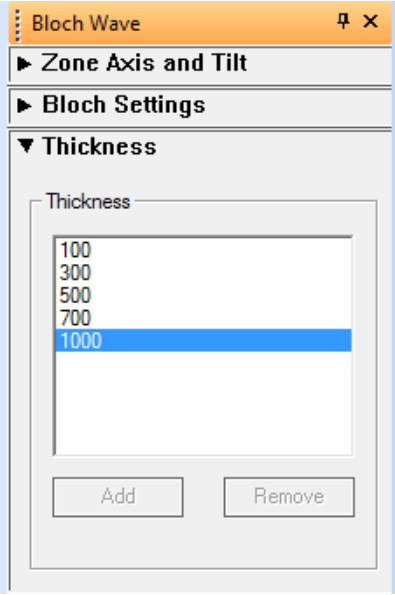
For the ***Circle*** and ***Precession*** modes the ***Width*** (in *mrad*) of the ring can be modified.

NOTE: Line specific settings. The ***Number of points*** has no effect on the lined width and determines the sampling (resolution along the line). The line width determined by the *convergence angle* – it is a segment which is the result of the intersection of an infinite line and the CBED disk.



The line slope related to the electron diffraction pattern axis, the line width and length are marked.

5.2.3 The Thickness dialog panel

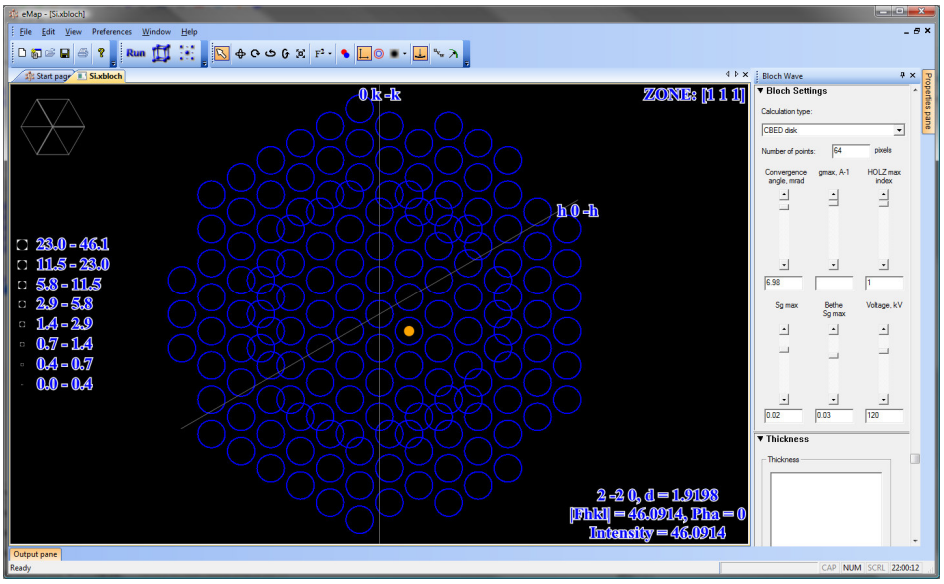


The **Thickness** dialog panel.

The **Thickness** dialog panel allows the user to control the current thickness value, and to add and remove thickness values to the list. The thickness list is always enabled. Changing the selection in the list will automatically change the ***calculated*** dynamical electron diffraction pattern. The thickness selection doesn't affect the diffraction pattern in ***preview mode*** (the mode with blue circles representing the spots, see next section).

5.3 Optimal Bloch settings

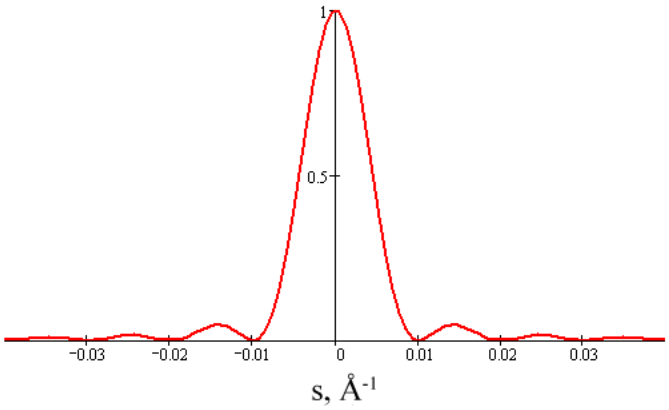
Consider the following example. The electron diffraction pattern of silicon along the [111] zone axis with current settings will be displayed as:



Some overlapping of reflections is due to large values of S_g.

The optimal settings such as the beam convergence angle, excitation error values S_g, maximum HOLZ number etc. can be controlled visually in run-time via the side docking panels.

NOTE: The S_g value can be related to the kinematical crystal thickness t and the kinematical extension of reflections in reciprocal space as $S_g = 1/t$.

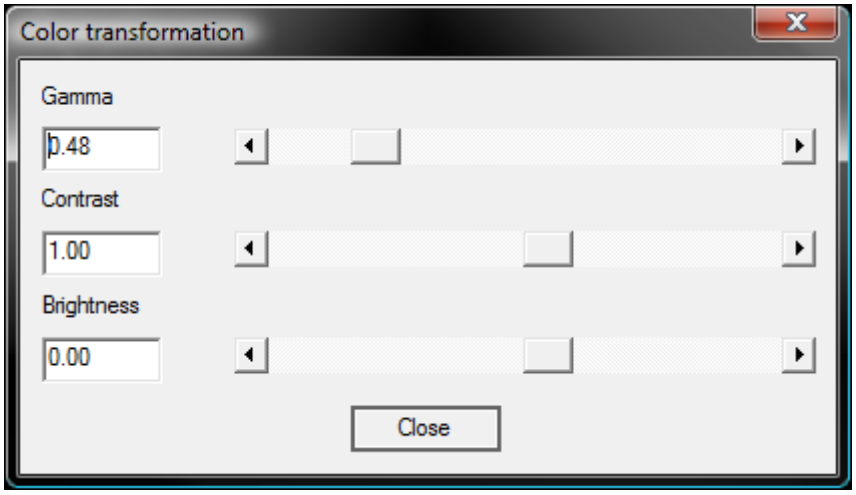


The user can modify the numbers in the dialog boxes or change them by dragging the corresponding scroll bars.

In the ***preview mode*** each blue circle corresponds to a CBED disk. Some information (such as *hkl*, *d* and kinematical F_{hkl} values) can be recalled by pointing the mouse to the centre of the corresponding disk. The information will be shown in the bottom-right corner.

5.4 Colour control

The following dialog will appear after pressing the colour control button  .



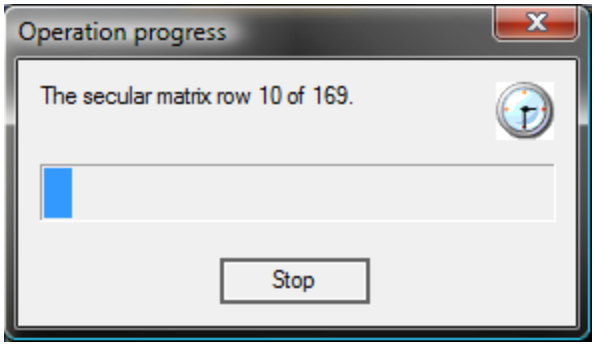
The user can modify the gamma, brightness and contrast values of the calculated dynamical electron diffraction pattern in order to increase the visual representation of some features on a diffraction pattern.

It has affect only on the ***calculated*** electron diffraction pattern.

6 Performing Bloch wave calculations

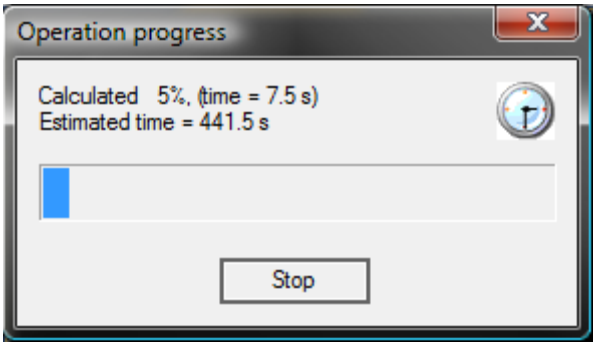
In order to start the Bloch calculations press the **Run** button on the *Bloch wave Simulator* toolbar. This button may be disabled if the previous calculated Bloch data hasn't been cleared or reset. In order to reset the data and be able to run new calculations press the **Create new document** button ( ).

When the calculations starts the following control dialog will appear:



The calculations can be stopped at any time by pressing the ***Stop*** button. Firstly the program will calculate the secular matrix while informing the user about the current row been calculated.

After that the program will start the matrix diagonalization procedure with the following dialog.



NOTE: the current time (in the first row) is exact, however the estimated (total) time is only an approximation and may vary.

7 Examples

The following dynamical electron diffraction patterns were calculated by the Bloch method using the *Bloch wave Simulator*. The conditions were:

Crystal: silicon;

Zone axis: [111]

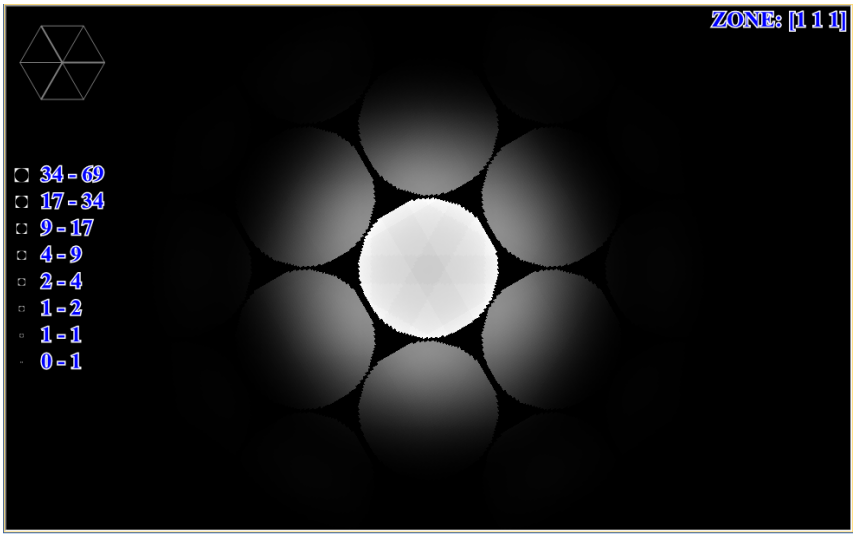
Voltage: 200 kV

CBED disk size: 64 pixels

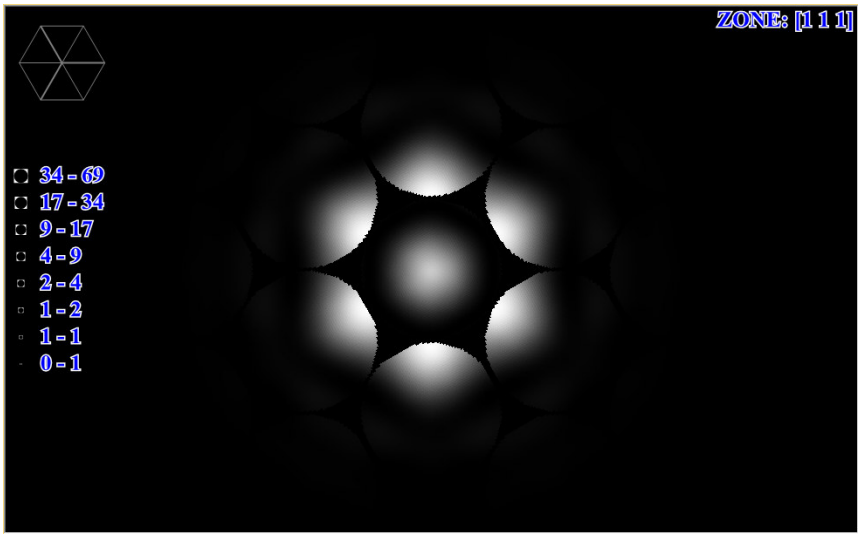
Convergence angle: 8 mrad

HOLZ included: 2

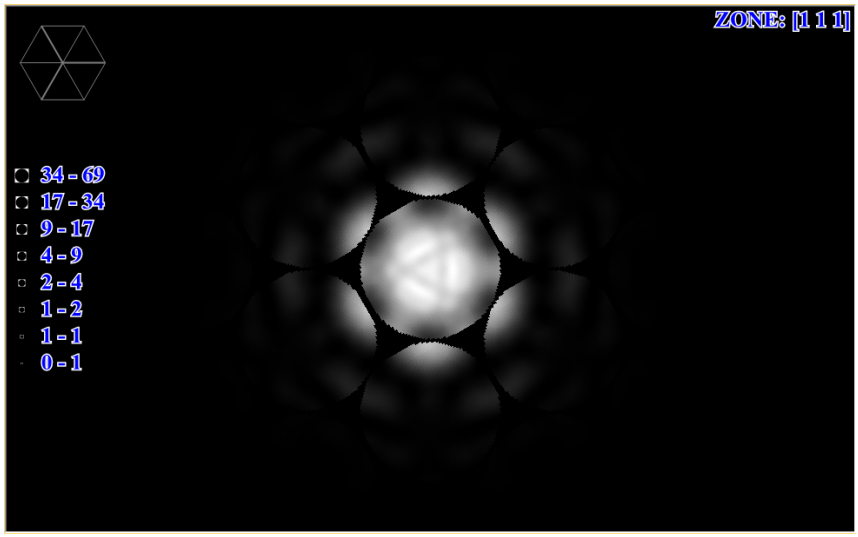
Thickness values: 100, 300, 500 and 1000 Å.


ZONE: [1 1 1]
34 - 69
17 - 34
9 - 17
4 - 9
2 - 4
1 - 2
1 - 1
0 - 1

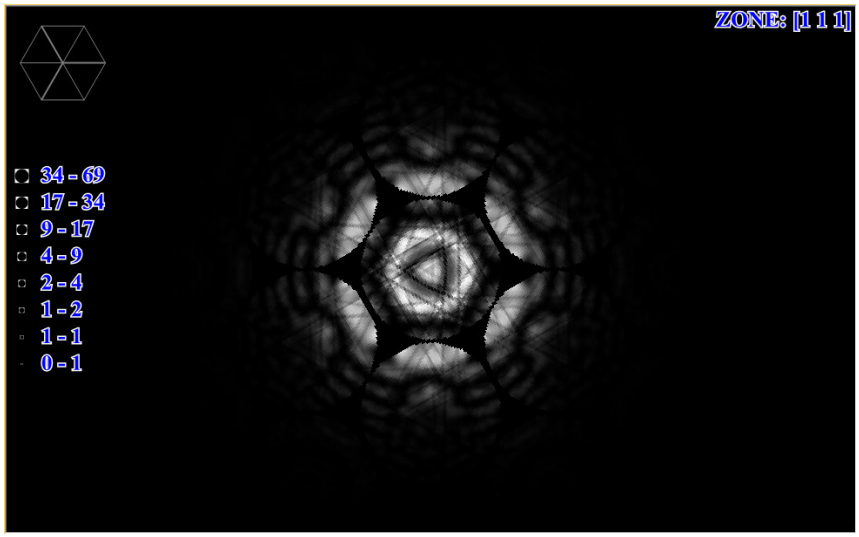
100 Å


ZONE: [1 1 1]
34 - 69
17 - 34
9 - 17
4 - 9
2 - 4
1 - 2
1 - 1
0 - 1

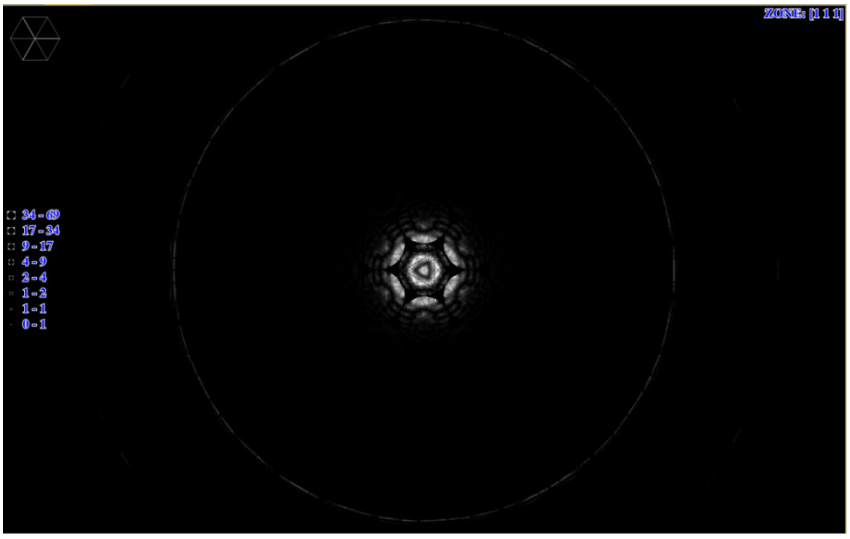
300 Å


ZONE: [1 1 1]
34 - 69
17 - 34
9 - 17
4 - 9
2 - 4
1 - 2
1 - 1
0 - 1

500 Å


ZONE: [1 1 1]
34 - 69
17 - 34
9 - 17
4 - 9
2 - 4
1 - 2
1 - 1
0 - 1

1000 Å



1000 Å, zoomed with FOLZ visible.

8 Suggested literature

1. **Z.L. Wang**. *Elastic and Inelastic Scattering in Electron Diffraction and Imaging*. Springer. 1995, 476 pp.
2. **E.J. Kirkland**. *Advanced Computing in Electron Microscopy*. Springer. 1998, 250 pp.
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4. **L.-M. Peng, S.L. Dudarev, M.J. Whelan.** *High-Energy Electron Diffraction and Microscopy*. Oxford University Press. 2004, 536 pp.